

# CURRICULUM VITAE

DR. THOMAS PROFFEN

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<http://www.researcherid.com/rid/B-3585-2009>

## EMPLOYMENT

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- since 2001      **Technical Staff Member** at Lujan Neutron Scattering Center, Los Alamos National Laboratory, USA.
- 1998 - 2001      **Research Associate** with Prof. S.J.L Billinge at the Department of Physics and Astronomy, Michigan State University, USA.
- 1995 - 1998      **Postdoctoral Fellow** with Dr. T.R. Welberry at the Research School of Chemistry, The Australian National University, Australia.
- 1992 - 1995      **Doctoral Fellow** with Prof. F. Frey at the Neutron Scattering Group, Department of Mineralogy and Crystallography, Ludwig Maximilians Universität (LMU), Munich, Germany.
- 1990 - 1994      **Assistant lecturer** (part time) "Mathematical methods in Crystallography" including a FORTRAN programming course, Department for Mineralogy and Crystallography, LMU.
- 1989                **Assistant** for the development of programs analyzing IR satellite images at the meteorological department, LMU.

## EDUCATION

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- 28 Jun 1995      **PhD (Dr. rer. nat.)** "Disorder and diffuse neutron and X-ray scattering from zirconia at temperatures up to 1500 K using newly designed experimental X-ray techniques" at Ludwig Maximilians Universität, Munich, Germany
- 04 Feb 1992      **Diploma (Physics)** "Disorder in CaO stabilized zirconia studied using diffuse neutron scattering from RT to 1750 K", at Ludwig Maximilians Universität, Munich, Germany
- 25 May 1983      **Abitur (High School Graduation)** at Helene-Lange Gymnasium, Rendsburg, Germany

## GRANTS

- 2007 - 2012 Work for Others Agreement with the National Institute of Advanced Industrial Science and Technology in Tsukuba, Japan on Hydrogen Storage Materials. (Total funding ~ US\$ 1,250,000)
- 2001 - 2004 Los Alamos National Laboratory LDRD grant: "Local Structure in Complex Materials". (Total funding ~ US\$ 525,000)
- 1995 - 1997 Research grant by Deutsche Forschungsgemeinschaft: "Disorder and Diffuse Scattering from Zirconia Doped with CaO and Y<sub>2</sub>O<sub>3</sub>".

## AWARDS

- 2009 Selected for the Leadership Development Initiative program of the Los Alamos National Laboratory's Experimental Science's Directorate.
- 2006 Los Alamos National Laboratory Women's Career Development Outstanding Mentoring Award.
- 2006 Los Alamos LAAP Award (for achievements as local chair of the American Conference on Neutron Scattering).
- 2005 Los Alamos LAAP Award (for achievements related to preparation for Lujan Center review by the Department of Energy).
- 2002 Los Alamos National Laboratory Individual Distinguished Performance Award.

## OFFICIAL FUNCTIONS

- since 2009 Communications Officer on the Executive Committee of the Neutron Scattering Society of America.
- since 2009 Member of the Communications Standing Committee of the American Crystallographic Association.
- since 2008 Member of the Los Alamos National Laboratory's Experimental Science's Directorate Promotion Committee.
- 2009 Organizer of the symposium "Quantitative Characterization of Nanostructured Materials" at the MRS spring meeting.
- 2007 Organizer of the transaction symposium at the Annual Meeting of the American Crystallographic Association.
- 2007 Local chair and member of the Program Committee of the American Conference on Neutron Scattering in Santa Fe.
- 2006-2010 Member of the Los Alamos National Laboratory Postdoc Committee (Chair of committee in 2009).

## OFFICIAL FUNCTIONS (CONT.)

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2005	Member of the Program Committee for the European Powder Diffraction Conference.
since 2004	Editor of <i>Zeitschrift für Kristallographie</i> .
since 2003	Member of the Instrument Advisory Team (IAT) for the disordered materials diffractometer (NOMAD) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
2003-2010	Member of the NeXus International Advisory Committee.
2002-2003	President of the Neutron Scattering Special Interest Group of the American Crystallographic Association.
since 2002	Member of the executive committee for the single crystal diffractometer (SCD) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
since 2001	Member of the Instrument Advisory Team (IAT) for the high-resolution powder diffractometer (POW-GEN3) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
2001-2003	Member of the LANSCE Materials Program Advisory Committee (PAC).
1998-2005	Responsible for development of difCIF, an extension of the Crystallographic Information File format to include diffuse scattering.

## OTHER ACTIVITIES

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- Frequent reviewer of papers for major scientific journals including Science, Physical Review Letters and Journal of the American Chemical Society.
- Reviewer of funding proposals of major funding agencies including the Office of Science of the Department of Energy and the European Commission's CORDIS program.
- Member of experimental proposal review committees of national user facilities including ISIS, NIST, LANSCE and SNS.
- Organizer of ~ 20 workshops on total scattering analysis.
- Served a judge for student presentations including the Los Alamos County Science Fair and Los Alamos National Laboratory Student Symposium.
- Engaged in outreach activities, frequent tour guide for the Lujan Neutron Scattering Center for groups ranging from school children to high level national and international visitors.
- Served as acting Lujan Neutron Scattering Center leader.
- Served on the Lujan Experiment Safety Review Committee.

## **MENTORSHIP**

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- Member of the thesis committee of Katharine Page (University of California Santa Barbara).
- Mentor of four postdocs and 20 graduate and undergraduate students.
- Supervision of ~ 80 students and postdocs visiting as users of the NPDF instrument.
- Served on the Rosen Thesis Award Committee.

## **MEMBERSHIPS**

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American Physical Society

American Crystallographic Association

Neutron Scattering Society of America

## **REFERENCES**

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Available upon request.

## LIST OF PUBLICATIONS (H FACTOR: 22)

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### Books and book chapters

- [1] K. PAGE, TH. PROFFEN, AND R.B. NEDER. Structure of Nanoparticles from Total Scattering. In E.J. MITTERMEIER, editor, *Modern Diffraction Methods*, Weinheim, October 2010. Wiley Verlag GmbH.
- [2] K. PAGE AND TH. PROFFEN. Nanoparticle Structure from Neutron Total Scattering: the Pair Distribution Function Approach. In A. HURD AND S. SINHA, editors, *Neutrons and Nanoscience*, New York, November 2010. Springer.
- [3] R.B. NEDER AND TH. PROFFEN. *Diffuse Scattering and Defect Structure Simulations: A cook book using the program DISCUS*. International Union of Crystallography Texts on Crystallography. Oxford University Press, November 2008.

### Peer reviewed papers

- [1] C. WURDEN, K.L. PAGE, A. LLOBET, C.E. WHITE, AND TH. PROFFEN. Extracting Differential Pair Distribution Functions unsing MIXSCAT. *J. Appl. Cryst.*, 2010. in press.
- [2] C.E. WHITE, J.L. PROVIS, TH. PROFFEN, D.P. RILEY, AND J.S.J. VAN DEVENTER. Combining density functional theory (DFT) and pair distribution function (PDF) analysis to solve the structure of metastable materials: the case of metakaolin. *Phys. Chem. Chem. Phys.*, 2010. in press.
- [3] M. FABIAN, E. SVAB, TH. PROFFEN, AND E. VERESS. Neutron diffraction and reverse Monte Carlo modelling of v-B<sub>2</sub>O<sub>3</sub> and 75B<sub>2</sub>O<sub>3</sub>25Na<sub>2</sub>O glasses. *J. Non-Cryst. Solids*, 356:441–446, 2010.
- [4] M.H. BRAGA, J.J.A. FERREIRA, J. SIEWENIE, TH. PROFFEN, S.C. VOGEL, AND L.L. DAEMEN. Neutron powder diffraction and first-principles computational studies of CuLi<sub>x</sub>Mg<sub>2-x</sub> (x=0.08), CuMg<sub>2</sub>, and Cu<sub>2</sub>Mg. *J. Solid State Chem.*, 183:10–19, 2010.
- [5] D. LOUCA, K. KAMAZAWA, AND TH. PROFFEN. Formation of local electric dipoles with no unique polar axis in Tb<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub>. *Phys. Rev. B*, 80:214406, 2009.
- [6] V.F. KRANAK, M.J. EVANS, L.L. DAEMEN, TH. PROFFEN, M.H. LEE, O.F. SANKEY, AND U. HÄUSERMANN. Structural and dynamic properties of the polyanionic hydrides SrAlGeH and BaAlGeH. *Sol. State Sci.*, 11:1847–1853, 2009.
- [7] V. KRAYZMAN, I. LEVIN, J.C. WOICIK, TH. PROFFEN, T.A. VANDERAHA, AND M. G. TUCKER. A combined fit of total scattering and extended X-ray absorption fine structure data for local structure determination in crystalline materials. *J. Appl. Cryst.*, 42:867–877, 2009.
- [8] R. UBIC, G. SUBODH, D. GOUT, M.T. SEBASTIAN, AND TH. PROFFEN. Crystal Structure of Sr<sub>0.4</sub>Ce<sub>0.4</sub>TiO<sub>3</sub> Ceramics. *Chem. Mater.*, 21:4706–4710, 2009.
- [9] B.C. MELOT, K. PAGE, R. SESHDARI, E.M. STOUDENMIRE, L. BALENTS, AND D.L. BERGMAN TH. PROFFEN. Magnetic frustration on the diamond lattice of the A-site magnetic spinels CoAl<sub>2-x</sub>Ga<sub>x</sub>O<sub>4</sub>: Lattice expansion versus site disorder. *Phys. Rev. B*, 80:104420, 2009.
- [10] H. KIM, A. KARKAMKAR, T. AUTREY, P. CHUPAS, AND TH. PROFFEN. Determination of structure and phase transition of light element nanocomposites in mesoporous silica: case study of NH<sub>3</sub>BH<sub>3</sub> in MCM-41. *J. Am. Chem. Soc.*, 131:13749–13755, 2009.
- [11] M.J. EVANS, V.F. KRANAK, F.J. GARCIA-GARCIA, G.P. HOLLAND, L.L. DAEMEN, TH. PROFFEN, M.H. LEE, O.F. SANKEY, AND U. HUSSELMANN. Structural and Dynamic Properties of BaInGeH - A Rare Solid State Indium Hydride. *Inorg. Chem.*, 48:5602–5604, 2009.
- [12] TH. PROFFEN AND H. KIM. Advances in Total Scattering Analysis. *J. Mater. Chem.*, 19:5078–5088, 2009.
- [13] L. MALAVASI, H. KIM, AND TH. PROFFEN. Local and average structures of the proton conducting Y-doped BaCeO<sub>3</sub> from neutron diffraction and neutron pair distribution function analysis. *J. Appl. Phys.*, 105:123519, 2009.
- [14] J. ROPKA, R. CERNY, V. PAUL-BONCOUR, AND TH. PROFFEN. Deuterium ordering in Laves phase deuteride YFe<sub>2</sub>D<sub>4.2</sub>. *J. Solid State Chem.*, 182:1907–1912, 2009.
- [15] E.E. RODRIGUEZ, A. LLOBET, TH. PROFFEN, B.C. MELOT, R. SESHDARI, P.B. LITTLEWOOD, AND A.K. CHEETHAM. The role of static disorder in negative thermal expansion in ReO<sub>3</sub>. *J. Appl. Phys.*, 105:114901, 2009.

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- [17] I. LEVIN, V. KRAYZMAN, J.C. WOICIK, J. KARAPETROVA, **TH. PROFFEN**, M.G. TUCKER, AND I.M. REANEY. Structural changes underlying the diffuse dielectric response in AgNbO<sub>3</sub>. *Phys. Rev. B*, 79:104113, 2009.
- [18] J.E. GREEDAN, D. GOUT, A.D. LOZANO-GORRIN, S. DERAHKSHAN, **TH. PROFFEN**, H.J. KIM, E. BOIN, AND S.J.L. BILLINGE. Local and average structures of the spin-glass pyrochlore Y<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub> from neutron diffraction and neutron pair distribution function analysis. *Phys. Rev. B*, 79:014427, 2009.
- [19] N. SUNDARAM, Y. JIANG, I.E. ANDERSON, D.P. BELANGER, C.H. BOOTH, F. BRIDGES, J.F. MITCHELL, **TH. PROFFEN**, AND H. ZHENG. Local Structure of La<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3</sub> determined from EXAFS and Neutron PDF studies. *Phys. Rev. Lett.*, 102:026401, 2009.
- [20] Y.-I. KIM, S. CADARS, R. SHAYIB, **TH. PROFFEN**, C.S. FEIGERLE, B.F. CHMELKA, AND R. SESADRI. Local structures of polar wurtzites Zn<sub>1-x</sub>Mg<sub>x</sub>O studied by Raman and <sup>67</sup>Zn/<sup>25</sup>Mg NMR spectroscopies and by total neutron scattering. *Phys. Rev. B*, 78:195205, 2008.
- [21] K. PAGE, T. KOLODIAZHNYI, **TH. PROFFEN**, A.K. CHEETHAM, AND R. SESADRI. Local structural origins of the distinct electronic properties of Nb-substituted SrTiO<sub>3</sub> and BaTiO<sub>3</sub>. *Phys. Rev. Lett.*, 101:205502, 2008.
- [22] K. PAGE, J. LI, R. SAVINELLI, H.N. SZUMILA, J. ZHANG, J. STALICK, **TH. PROFFEN**, S.L. SCOTT, AND R. SESADRI. Reciprocal-Space and Real-Space Neutron Investigation of Nanostructured Mo<sub>2</sub>C and WC. *J. Mater. Chem.*, 10:1499–1510, 2008.
- [23] L. MALAVASI, H. KIM, **TH. PROFFEN**, AND G. FLOR. New Insight into the Properties of Proton Conducting Oxides from Neutron Total Scattering. *Chem. Phys. Chem.*, 9:2309–2312, 2008.
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- [26] T. WILSON, B. CLAUSEN, **TH. PROFFEN**, J. ELLE, AND B. BROWN. In-Situ Neutron Scattering Measurement of Stress-Strain Behavior of a Bulk Metallic Glass. *Metal. and Mater. Trans. A*, 39:1942–1946, 2008.
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- [28] R. UBIC, G. SUBODH, M.T. SEBASTIAN, D. GOUT, AND **TH. PROFFEN**. Structure of compounds in the Sr<sub>1-3x/2</sub>Ce<sub>x</sub>TiO<sub>3</sub> Homologous Series. *Chem. Mater.*, 20:3127–3133, 2008.
- [29] D. GOUT, O. GOURDON, E.D. BAUER, F. RONNING, J.D. THOMPSON, AND **TH. PROFFEN**. An Experimental and Theoretical Study of the Variation of 4f hybridization across the La<sub>1-x</sub>Ce<sub>x</sub>In<sub>3</sub> series. *Inorg. Chem.*, 47:2569–2577, 2008.
- [30] M. WOJDYR, Y. MO, E. GRZANKA, S. STELMAKH, S. GIERLOTKA, **TH. PROFFEN**, T.K. ZERDA, B. PALOSZ, AND I. SZLUFARSKA. Transition of nc-SiC Powder Surface into Grain Boundaries during Sintering by Molecular dynamics Simulaton and Neutron Powder Diffraction. *Z. Krist.*, S26:255–260, 2007.
- [31] E.S. BOZIN, X. QUI, R.J. WORHATCH, G. PAGLIA, M. SCHMIDT, P.G. RADAELLI, J.F. MITCHELL, T. CHATTERJI, **TH. PROFFEN**, AND S.J.L. BILLINGE. Atomic Pair Distribution Function Study of the Jahn-Teller Transition in La<sub>1-x</sub>Ca<sub>x</sub>MnO<sub>3</sub>. *Z. Krist.*, S26:429–434, 2007.
- [32] K. PAGE, C.S. SCHADE, J. ZHANG, P.J. CHUPAS, K.W. CHAPMAN, **TH. PROFFEN**, A.K. CHEETHAM, AND R. SESADRI. Preparation and Characterization of Pd<sub>2</sub>Sn Nanoparticles. *Mat. Res. Bull.*, 42:1969–1975, 2007.
- [33] D.J. WILLAMS, L.L. DAEMEN, S.C. VOGEL, AND **TH. PROFFEN**. Temperature dependence of the crystal structure of  $\alpha$ -AgSCN by powder neutron diffraction. *J. Appl. Cryst.*, 40:1039–1043, 2007.
- [34] M. FABIAN, P. JOVARI, G.Y. MESZAROS, E. SVAB, **TH. PROFFEN**, AND E. VERESS. Network Structure of 0.7SiO<sub>2</sub>-0.3Na<sub>2</sub>O glass from Neutron and X-ray Diffraction and RMC Modelling. *J. Phys.: Cond. Matt.*, 19:355209, 2007.
- [35] T. WILSON, B. CLAUSEN, **TH. PROFFEN**, J. ELLE, AND B. BROWN. In-Situ Neutron Scattering Measurement of Stress-Strain Behavior of a Bulk Metallic Glass. *Metal. and Mater. Trans. A*, 2007.
- [36] C.L. FARROW, P. JUHAS, J.W. LIU, D. BRYNDIN, J. BLOCH, **TH. PROFFEN**, AND S.J.L. BILLINGE. PDFfit2 and PDFgui: Computer Programs for Studying Nanostructure in Crystals. *J. Phys.: Condens. Matter*, 19:335219, 2007.

- [37] K. PAGE, M.W. STOLTZFUS, Y.-I. KIM, TH. PROFFEN, P.M. WOODWARD, A.K. CHEETHAM, AND R. SESHADRI. Local Atomic Ordering in BaTaO<sub>2</sub>N Studied by Neutron Pair Distribution Function Analysis and Density Functional Theory. *Chem. Mater.*, 19:4037–4042, 2007.
- [38] I.-K. JEONG, N. HUR, AND TH. PROFFEN. High temperature structural evolution of hexagonal multiferroic YMnO<sub>3</sub> and YbMnO<sub>3</sub>. *J. Appl. Cryst.*, 40:730–734, 2007.
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- [41] L. MALAVASI, H. KIM, S.J.L. BILLINGE, TH. PROFFEN, C. TEALDI, AND G. FLOR. Nature of the Monoclinic to Cubic Phase Transition in the Fast Oxygen Ion Conductor La<sub>2</sub>Mo<sub>2</sub>O<sub>9</sub> (LAMOX). *J. Am. Chem. Soc.*, 129:6903–6907, 2007.
- [42] M. FEUERBACHER, C. THOMAS, J.P.A. MAKONGO, S. HOFFMANN, W. CARRILLO-CABRERA, R. CARDOSO, YU. GRIN, G. KREINER, J.-M. JOUBERT, TH. SCHENK, J. GASTALDI, H. NGUYEN-THI, N. MANGELINCK-NOL, B. BILLIA, P. DONNADIEU, A. CZYRSKA-FILEMONOWICZ, A. ZIELINSKA-LIPIEC, B. DUBIEL, TH. WEBER, P. SCHAUB, G. KRAUSS, V. GRAMLICH, J. CHRISTENSEN, S. LIDIN, D. FREDRICKSON, M. MIHALKOVIC, W. SIKORA, J. MALINOWSKI, S. BRÜHNE, TH. PROFFEN, W. ASSMUS, M. DE BOISSIEU, F. BLEY, J.L. CHEMIN, J. SCHREUER, AND W. STEURER. The Samson phase,  $\beta$ -Mg<sub>2</sub>Al<sub>3</sub>, revisited. *Z. Krist.*, 222:259–288, 2007.
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- [44] G. CAMPI, TH. PROFFEN, X. QIU, E.S. BOZIN, S.J.L. BILLINGE, S. AGRESTINI, N.L. SAINI, AND A. BIANCONI. Local Lattice Dynamics in the Mg<sub>0.5</sub>Al<sub>0.5</sub>B<sub>2</sub> Superconductor. *J. Supercond. Nov. Magn.*, 2007.
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## Non reviewed papers

- [1] S.D. MILLER, K.W. HERWIG, S. REN, S.S. VAZHKUDAI, P.R. JEMIAN, S. LUITZ, A.A. SALNIKOV, I. GAPO-NENKO, TH. PROFFEN, P. LEWIS, AND M.L. GREEN. Data Management and Its Role in Delivering Science at DOE BES User Facilities Past, Present, and Future. *Journal of Physics: Conference Series*, 180:012049, 2009.
- [2] TH. PROFFEN, K.L. PAGE, R. SESHADRI, AND A.K. CHEETHAM. Pair Distribution Function for Nanoparticle Studies. *Los Alamos Science*, 30:161–164, 2006.
- [3] TH. PROFFEN AND T. EGAMI. Unraveling the True Atomic Structures of Exotic Oxides. *Los Alamos Science*, 30:152–160, 2006.
- [4] TH. PROFFEN. Total Scattering: The Key to the True Atomic Structure of Complex Materials. *Nuclear Weapons Journal*, 2005.
- [5] TH. PROFFEN. Calculating the Pair Distribution Function from a Structural Model. *Commission on Crystallographic Computing of the International Union of Crystallography, Newsletter number 5*, 2005.
- [6] S. J. L. BILLINGE, V. PETKOV, AND TH. PROFFEN. Structure on different length scales from powder diffraction: the real-space pair distribution function (PDF) technique. *Commission on Powder Diffraction of the International Union of Crystallography, Newsletter number 24*, 2000.

## Invited talks and organized workshops

- [1] TH. PROFFEN. Total Scattering Studies of Metal Hydrides. *invited talk - Hydrogen Forum, Tokyo, JAPAN*, February 2010.
- [2] TH. PROFFEN. Unlocking the 'True' Structure of Complex Materials using Total Scattering. *invited talk - TMS meeting, Seattle, WA*, February 2010.
- [3] TH. PROFFEN. Total scattering: Experiments, modeling and the future. *invited seminar - CNLS, LANL, Los Alamos, NM*, January 2010.
- [4] TH. PROFFEN. Disordered crystals - Diffuse scattering to the rescue. *invited talk - Pittsburgh Diffraction Conference, Athens, GA*, October 2009.
- [5] TH. PROFFEN. R-Dependent Refinements: An Alternative to RMC? *invited talk - RMC4 Conference, Budapest, HUNGARY*, October 2009.
- [6] TH. PROFFEN. Local structure and crystallographic phase transitions. *invited talk - Annual Meeting of American Crystallographic Association; Toronto; CANADA*, July 2009.
- [7] TH. PROFFEN. Total Scattering. *invited lecture - LANSCE Neutronschool; Los Alamos; NM*, July 2009.
- [8] TH. PROFFEN. Total Scattering: The Key to Local and Medium Range Structure of Materials. *invited seminar - Chemistry Department, University of Sussex, Brighton, UK*, June 2009.
- [9] TH. PROFFEN. Total Scattering: The Key to Local and Medium Range Structure of Materials. *invited talk - TMS meeting, San Francisco, CA*, February 2009.
- [10] TH. PROFFEN. Diffuse Streuung - der Schlüssel zur strukturellen Fehlordnung komplexer Systeme. *invited seminar - University of Frankfurt, Frankfurt, GERMANY*, December 2008.
- [11] TH. PROFFEN. Total Scattering Tutorial. *invited tutorial - MRS meeting, Boston, MA*, November 2008.
- [12] TH. PROFFEN. Total Scattering: The Key to Local and Medium Range Structure of Materials. *invited seminar - UCSB, Santa Barbara, CA*, November 2008.
- [13] TH. PROFFEN. Total Scattering. *invited lecture - ORNL Neutronschool; Oak Ridge; TN*, October 2008.
- [14] TH. PROFFEN. Simulation of defect structures and diffuse scattering. *invited lectures and practicals - DISCUS workshop, Erlangen, GERMANY*, September 2008.
- [15] TH. PROFFEN. Understanding the Local Structure of Hydrogen Storage Materials.. *invited plenary talk - Third Annual NEDO/AIST/LANL Workshop, San Diego, CA*, September 2008.
- [16] TH. PROFFEN. Total Scattering: The Key to Local and Medium Range Structure of Materials. *invited talk - European Powder Diffraction Conference, Warsaw, POLAND*, September 2008.
- [17] TH. PROFFEN. Elastic Scattering / Total Scattering. *invited lectures - LANSCE Neutronschool; Los Alamos; NM*, July 2008.

- [18] **TH. PROFFEN.** Modeling of PDF data. *Workshop - British Crystallographic Meeting, York, UK*, March 2008.
- [19] **TH. PROFFEN.** Total Scattering: The Key to Local and Medium Range Structure of Materials. *invited talk - British Crystallographic Meeting, York, UK*, March 2008.
- [20] **TH. PROFFEN.** Total neutron scattering to obtain a 'complete' structural finger print of nano-particles. *invited talk - German Crystallographic Meeting, Erlangen, GERMANY*, March 2008.
- [21] **TH. PROFFEN.** Total Neutron Scattering: State of the Art. *invited talk - PDF workshop, NIST, Gaithersburg, MD*, February 2008.
- [22] **TH. PROFFEN.** Total Neutron Scattering: The Key to Local and Medium Range Structure of Complex Materials. *invited talk - International Symposium on Neutron Scattering, Mumbai, INDIA*, January 2008.
- [23] **TH. PROFFEN.** Total Scattering: The Key to Local and Medium Range Structure of Complex Materials. *invited talk - International Workshop on Structural Analyses Bridging over between Amorphous and Crystalline Materials, Tokai, JAPAN*, January 2008.
- [24] **TH. PROFFEN.** Understanding short- and medium range order in materials using total scattering. *invited seminar - Physics Department, University of Virginia, Charlottesville, VA*, November 2007.
- [25] **TH. PROFFEN.** Neutron Diffraction and Local Structure Determination Capabilities at the Lujan Neutron Scattering Center. *invited talk - Workshop on Hydrogen Storage Materials, Tokyo, JAPAN*, October 2007.
- [26] **TH. PROFFEN.** Understanding short- and medium range order in materials using total scattering. *invited lecture - Department of Engineering Sciences University Duisburg-Essen, Duisburg, GERMANY*, October 2007.
- [27] **TH. PROFFEN.** Modeling of total scattering data. *invited talk - Workshop: Total scattering Pair Distribution Function analysis using X-rays and neutrons: powder diffraction and complementary techniques, Grenoble, FRANCE*, October 2007.
- [28] **TH. PROFFEN.** Understanding short- and medium range order in materials using total scattering. *invited seminar - Materials Research Laboratory, University of California Santa Barbara, Santa Barbara, CA*, October 2007.
- [29] **TH. PROFFEN.** Understanding Short- and Medium Range Order in Materials Using Total Scattering. *invited talk - Denver X-ray conference; Colorado Springs; CO*, July 2007.
- [30] **TH. PROFFEN.** Diffraction, Bragg peaks and total scattering what does it mean ? *invited lecture - LANSCE Neutronschool; Los Alamos; NM*, July 2007.
- [31] **TH. PROFFEN.** Total scattering: the key to the local and medium range structure of complex materials. *invited talk - Canadian Chemistry Conference; Winnipeg; CANADA*, May 2007.
- [32] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited lecture and workshop - Canadian Powder Diffraction Workshop; Trois-Rivieres; CANADA*, May 2007.
- [33] **TH. PROFFEN.** Total neutron scattering: the key to the local and medium range structure of complex materials. *invited talk - Argonne National Laboratory Users Meeting, Argonne, IL*, May 2007.
- [34] **TH. PROFFEN.** Understanding short- and medium range order in materials using total neutron scattering. *invited seminar - Pacific Northwest National Laboratory, Richland, WA*, April 2007.
- [35] **TH. PROFFEN.** Total Scattering and Nanoparticles: Experiments and Modeling. *invited presentations - Advanced Workshop on Nanomaterials, Trieste, ITALY*, January 2007.
- [36] **TH. PROFFEN.** Analysis of Disordered Materials Using Total Scattering and the Atomic Pair Distribution Function. *invited presentation - MSA workshop, Emeryville, CA*, December 2006.
- [37] **TH. PROFFEN.** Characterizing complex materials using total neutron scattering. *invited presentation - Understanding Materials: The Role of the Lujan Neutron Scattering Center ; Los Alamos; NM*, November 2006.
- [38] **TH. PROFFEN.** NPDF Users Interface & Control. *invited presentation - Spallation Neutron Source; Oak Ridge; TN*, October 2006.
- [39] **TH. PROFFEN.** Diffraction, Bragg peaks and total scattering what does it mean ? *invited seminar - University of Tennessee; Knoxville; TN*, October 2006.
- [40] **TH. PROFFEN.** PDFIT and DISCUS: Unter der Motorhaube. *invited talk - European Powder Diffraction Conference; Geneva; SWITZERLAND*, September 2006.
- [41] **TH. PROFFEN.** A 'Complete' Structural Fingerprint of Nanoparticles . *invited talk - European Powder Diffraction Conference; Geneva; SWITZERLAND*, September 2006.
- [42] **TH. PROFFEN.** Total scattering: The key to the local and medium range structure of complex materials . *invited talk - Annual Meeting of the American Crystallographic Association; Honolulu; HI*, July 2006.

- [43] **TH. PROFFEN.** State of the NeXus file format. *invited talk - imgCIF workshop; Honolulu; HI*, July 2006.
- [44] **TH. PROFFEN.** Diffraction, Bragg peaks and total scattering what does it mean ? *invited seminar - LANSCE student seminar series; Los Alamos; NM*, July 2006.
- [45] **TH. PROFFEN.** Diffraction, Bragg peaks and total scattering what does it mean ? *invited lecture - LANSCE Neutronschool; Los Alamos; NM*, May 2006.
- [46] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited lecture and workshop - Canadian Powder Diffraction Workshop; Waterloo; CANADA*, May 2006.
- [47] **TH. PROFFEN.** From Crystalline to Amorphous: NPDF & Total Scattering Used as Universal Local Structural Probe. *invited seminar - ANSTO; Lukas Heights; AUSTRALIA*, April 2006.
- [48] **TH. PROFFEN.** From Crystalline to Amorphous: NPDF & Total Scattering Used as Universal Local Structural Probe. *invited seminar - University of California; Santa Cruz; CA*, November 2005.
- [49] **TH. PROFFEN.** Total Neutron Scattering: The Key Understanding Complex Materials. *invited talk - Multiferroics workshop; Los Alamos; NM*, November 2005.
- [50] **TH. PROFFEN.** Internal Strain Measurements in Bulk Metallic Glasses (BMG) and BMG Composites using Pair Distribution Function Analysis . *invited talk - MECASENS III; Santa Fe; NM*, October 2005.
- [51] **TH. PROFFEN.** Total neutron scattering to obtain a 'complete' structural finger print of nano-particles. *invited talk - SNS/HIFR Users Group Meeting; Oak Ridge; TN*, October 2005.
- [52] **TH. PROFFEN AND R.B. NEDER.** DISCUS, Diffuse Scattering and Disorder Simulation. *Workshop as part of IUCr XX software fayre; Florence; ITALY*, August 2005.
- [53] **TH. PROFFEN.** Pair Distribution Function Analysis: Data modeling. *invited talk - Annual Meeting of the American Crystallographic Association; Orlando; FL*, June 2005.
- [54] **TH. PROFFEN.** Total Neutron Scattering: The Key to the Local and Medium Range Structure of Complex Materials. *invited talk - Annual Meeting of the American Crystallographic Association; Orlando; FL*, June 2005.
- [55] **TH. PROFFEN.** From Crystalline to Amorphous: NPDF & Total Scattering Used as Universal Local Structural Probe. *invited seminar - State University of New York Stony Brook; Stony Brook; NY*, January 2005.
- [56] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited talk - NOMAD workshop; Oak Ridge; TN*, November 2004.
- [57] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - University Augsburg; Augsburg; GERMANY*, September 2004.
- [58] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - University Würzburg; Würzburg; GERMANY*, September 2004.
- [59] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - University Frankfurt; Frankfurt; GERMANY*, September 2004.
- [60] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited talk - 22nd European Crystallographic Meeting; Budapest; HUNGARY*, August 2004.
- [61] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - Technical University Darmstadt; Darmstadt; GERMANY*, August 2004.
- [62] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - T division; Los Alamos National Laboratory; Los Alamos; NM*, June 2004.
- [63] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited talk - DOE workshop on Neutrons in Chemistry; Airlie; VA*, June 2004.
- [64] **TH. PROFFEN AND S.J.L. BILLINGE.** Local Atomic Structure Using Neutron Pair Distribution Function Analysis. *Workshop as part of ACNS meeting; College Park; MD*, June 2004.
- [65] **TH. PROFFEN.** High resolution neutron powder diffractometry: NPDF at the Lujan Center . *invited talk - International Workshop on Time-of-Flight Diffraction in Reactor Sources: Review of EXED at HMI; Hahn-Meitner Institut; Berlin; GERMANY*, May 2004.
- [66] **TH. PROFFEN.** Time-of-Flight Powder Diffraction Data Analysis at the Lujan Neutron Scattering Center. *invited talk - IPNS; Argonne; IL*, May 2004.
- [67] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - New Mexico State University; Las Cruces; NM*, April 2004.

- [68] **TH. PROFFEN.** Local structure: the key to understanding complex materials. *invited talk - DELFS meeting; Santa Fe; NM*, March 2004.
- [69] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited seminar - University of Tennessee; Knoxville; TN*, January 2004.
- [70] **TH. PROFFEN.** From Crystalline to Amorphous: Total Scattering Used as Universal Local Structural Probe. *invited talk - Glass and Optical Materials Division Fall Meeting of the American Ceramic Society; Corning; NY*, October 2003.
- [71] **TH. PROFFEN.** Probing the local structure of real materials using the total neutron scattering approach. *invited seminar - FRM-II; Technical University Munich, Munich; GERMANY*, June 2003.
- [72] **TH. PROFFEN AND T.R. WELBERRY.** Monte Carlo based modelling of single crystal diffuse scattering. *invited talk - Workshop on Single Crystal Diffuse Scattering at Pulsed Neutron Sources; Argonne National Laboratory; Argonne; IL*, June 2003.
- [73] **TH. PROFFEN AND Y. ZHAO.** Neutron diffraction of the structure of fillers. *invited talk - Meeting of Rubber Division of American Chemical Society; San Fransico; CA*, April 2003.
- [74] **TH. PROFFEN AND S.J.L. BILLINGE.** Structural studies of disordered materials using pair distribution functions derived from neutron scattering data. *Workshop as part of NICEST symposium; Oak Ridge; TN*, March 2003.
- [75] **TH. PROFFEN.** Probing the local structure of real materials using the total neutron scattering approach. *invited seminar - Central Michigan University; Mt. Pleasant; MI*, January 2003.
- [76] **TH. PROFFEN.** Getting more from your diffraction pattern: Information beyond the average structure. *invited seminar - USRA/NASA-Marshall Space Flight Center; Huntsville; AL*, December 2002.
- [77] **TH. PROFFEN.** Obtaining structural information from real materials: the atomic pair distribution function. *invited talk - American Chemical Society Rocky Mountain Regional Meeting; Albuquerque; NM*, October 2002.
- [78] **TH. PROFFEN.** Getting more from your diffraction pattern: the atomic pair distribution function. *invited seminar - NIST Center for Neutron Research; Gaithersburg; MD*, November 2002.
- [79] **TH. PROFFEN.** Getting more from your diffraction pattern: the atomic pair distribution function. *invited seminar - California Institute of Technology; Pasadena; CA*, June 2002.
- [80] **TH. PROFFEN, V. PETKOV, S.J.L. BILLINGE, AND T. VOGT.** Chemical short-range-order information obtained from powder diffraction. *invited talk - Annual Meeting of the American Crystallographic Association; San Antonio; TX*, May 2002.
- [81] **TH. PROFFEN.** Getting more from your diffraction pattern: Information beyond the average structure. *invited seminar - Center for Catalytic Science and Technology, University of Delaware; Newark; DE*, January 2002.
- [82] **TH. PROFFEN.** Upgrade of the Neutron Powder Diffractometer NPD at the Manuel Lujan Jr. Neutron scattering center. *invited seminar - SNS division; Argonne National Laboratory; Argonne; IL*, October 2001.
- [83] **TH. PROFFEN.** Getting more from your diffraction pattern: Information beyond the average structure. *invited talk - 20th European Crystallographic Meeting; Krakow; Poland and 5th LANSCE Users Group Meeting; Los Alamos; NM*, August 2001.
- [84] **TH. PROFFEN, S.J.L. BILLINGE, AND V. PETKOV.** Real-Space Pair Distribution Function Methods. *Workshop held during Annual Meeting of the American Crystallographic Association; Los Angeles; CA*, July 2001.
- [85] **TH. PROFFEN.** Teaching Diffraction Using Computer Simulations over the Internet. *invited talk - Annual Meeting of the American Crystallographic Association; Los Angeles; CA*, July 2001.
- [86] **TH. PROFFEN.** Analyse der Paarverteilungsfunktion : Informationen jenseits der gemittelten Struktur. *invited seminar - University München; GERMANY*, December 1999.
- [87] **TH. PROFFEN AND S.J.L. BILLINGE.** Introduction into PDF Analysis. *Workshop held at Michigan State University; East Lansing; MI*, September 1999.
- [88] **TH. PROFFEN AND R.B. NEDER.** Why bother with an experiment ? Simulating crystals as a teaching tool and to analyze defect structures. *Workshop held during IUCr meeting in Glasgow; UK*, August 1999.
- [89] **TH. PROFFEN.** Fehlordnung, diffuse Streuung und die 'Pair Distribution Function'. *invited seminar - University Würzburg, GERMANY*, December 1998.
- [90] **TH. PROFFEN.** DISCUS 3.0, a Universal Program for Diffuse Scattering and Defect Structure Simultion. *invited seminar - University Lausanne; SWITZERLAND*, March 1997.
- [91] **TH. PROFFEN.** Reverse Monte Carlo: A General Method to Analyze Diffuse Scattering from Single Crystals ? *invited seminars - ETH Zürich and U München and TU Braunschweig; GERMANY*, February/March 1997.
- [92] **TH. PROFFEN.** Analysis of the Diffuse Neutron and X-ray Scattering of Stabilized Zirconia using the Reverse Monte Carlo Method. *invited talk - International Conference on Neutron Scattering; Toronto; CANADA*, August 1997.

## Computer programs

- [1] C. WURDEN, K.L. PAGE, A. LLOBET, C.E. WHITE, AND **TH. PROFFEN**. **MIXSCAT**: Program to Extract Differential Pair Distribution Functions from X-ray and Neutron Data, 2010.
- [2] C.L. FARROW, P. JUHAS, J.W. LIU, D. BRYNDIN, J. BLOCH, **TH. PROFFEN**, AND S.J.L. BILLINGE. **PDFgui**: Full Profile Structural Refinement of the Atomic Pair Distribution Function, 2007.
- [3] **TH. PROFFEN**. **NXproc**: Program for Analysis and Reduction of Time-of-Flight Powder Diffraction Data, 2002.
- [4] P.F. PETERSON, M. GUTMANN, **TH. PROFFEN**, AND S.J.L. BILLINGE. **PDFgetN**: A Data Analysis Package for Obtaining the Atomic Pair Distribution Function from Neutron Data, 2000.
- [5] **TH. PROFFEN** AND R.B. NEDER. **DISCUS**: Diffuse Scattering and Defect Structure Simulations, 1999. Homepage: <http://discus.sourceforge.net>.
- [6] **TH. PROFFEN** AND S.J.L. BILLINGE. **PDFFIT**: Full Profile Structural Refinement of the Atomic Pair Distribution Function, 1999.
- [7] **TH. PROFFEN**. **KUPLOT**: General Data Analysis and Plotting, 1999.
- [8] **TH. PROFFEN**. **PWID**: Extracting Peak Widths from the Atomic Pair Distribution Function, 1999.
- [9] I.K. JEONG, J. THOMPSON, **TH. PROFFEN**, V. PETKOV, AND S.J.L. BILLINGE. **PDFgetX**: A Data Analysis Package for Obtaining the Atomic Pair Distribution Function from X-ray Data, 1999.
- [10] **TH. PROFFEN** AND T.R. WELBERRY. **FOURDEM**: A Demonstration Program for Fourier Synthesis (multiple platforms), 1997.
- [11] **TH. PROFFEN**. **DK**: Data Reduction for Q-Scans on Diffractometer at D3 Beamline at HASYLAB, Hamburg, 1995.
- [12] **TH. PROFFEN** AND R.B. NEDER. **DOMFIT**: Refinement of Diffuse Scattering based on Correlated Microdomains, 1994.
- [13] R.B. NEDER AND **TH. PROFFEN**. **MAN2**: Control Software for Neutron Four Circle Diffractometer MAN2, 1994.
- [14] R.B. NEDER AND **TH. PROFFEN**. **MPAUS**: Processing and Analysis of 2D Detector Data., 1994.